Literature review of pressure-induced amorphization

Feng Wang

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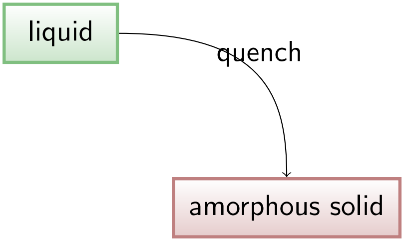
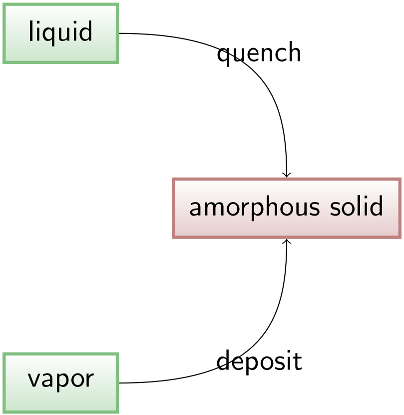
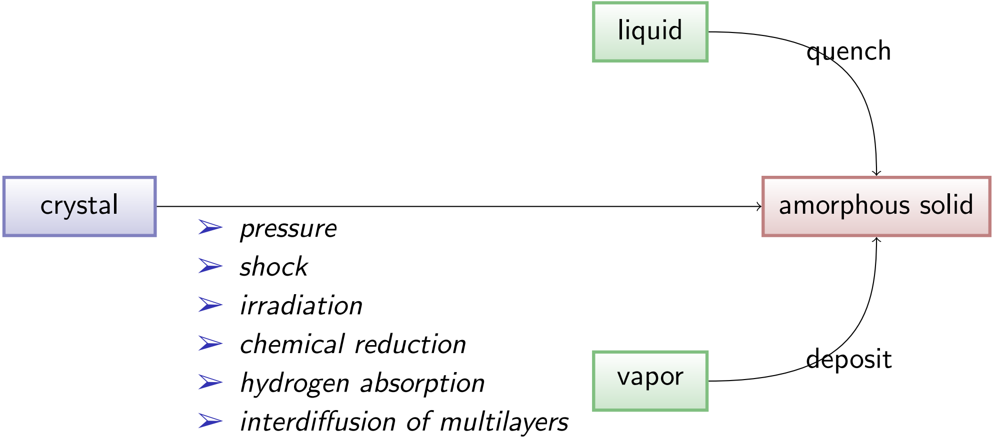
Approaches to obtaining amorphous solids



Approaches to obtaining amorphous solids



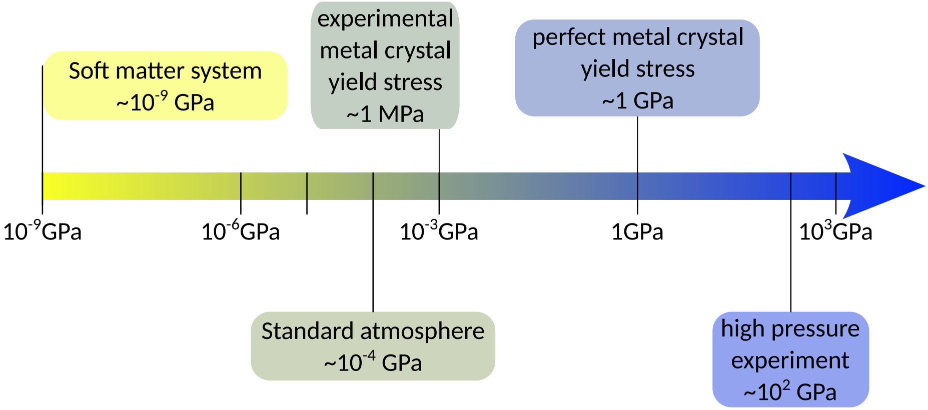
Approaches to obtaining amorphous solids



Converting crystals to amorphous solids

- **Pressured-induced amorphization (PIA)**
  - most cases are increasing pressure, i.e. compression
  - depressurization amorphization: e.g. boron carbide (B_4C) PRL 102, 075505 (2009)
- **Shock**
  - e.g. Boron carbide B_4C, PRL 102, 075505 (2009)
  - it may related to quenching or pressured-induced amorphization
- **Irradiation** (accumulating defects)
  - Cubic silicon carbide (SiC) (has very rich and interesting properties). PRL 111, 155501 (2013)
  - fcc Si sublattice is unstable if C is removed. This intrinsic mechanical instability drives the amorphization. The obtained $g(r)$ is very similar to the one from quenching a liquid.
  - For single component system (e.g. LJ fcc crystal), amorphization won't happen till the accumulated interstitial concentration $> 25\%$. RPL 59, 2760 (1987)
- Instability of metastable solid solution Mo Li, PRL 70, 1120 (1993)

Pressure scale



Facts

lower mantle: 24 GPa - 136 GPa
the core of the sun: 3 x10^{7} GPa
neutron star: 10^{22} - 10^{25} GPa

Materials showing PIA

Mainly are **tetrahedrally coordinated materials**. PRB 71, 224119 (2005)

- Ice I_h Nature 310, 393 (1984); Nature 384, 546 (1996);
  - low density amorphous ice (LDA): usually from vapor-deposition
  - high density amorphous ice (HDA): compress ice I_h at 77 K to 1.6 GPa, or compress LDA at 77 K to 0.5 GPa
  - very high density amorphous ice: warm HDA to 160K 77 K at $\sim$2 GPa
- silica SiO_2: coesite PNAS 114, 12894 (2017); quartz Treatise on Geophysics (Second Edition) (2015); Nature 334, 52 (1988); PRL 69, 1387 (1992)
- GeO_2 PRL 93, 115502 (2004)
- $Ge_2Sb_2Te_5$ PNAS 108, 10410 (2011)
- α-berlinite $AlPO_4$ Science 255, 1559 (1992)
- boron carbide (B_4C): one of the superhard materials, it also has very low density, used as armor ceramic
- Zirconium tungstate ZrW_2O_8: the most studied negative thermal expansion material Science 280, 886 (1998)
- SnI_4 JCP 143 164508 (2015)
- clathrate hydrates JCP 94, 623 (1991)
- zeolite silica (microporous: pores diameter $<$ 2nm) Nature 369, 724 (1994)
- *pressure-release amorphization: perovskite-structured modification of $CaSiO_3$, one of the main minerals of the Earth's lower mantle, which at ambient conditions turns to a glass within a few hours.* Treatise on Geophysics (Second Edition) (2015)
- Progress in Materials Science 40, 1 (1996) gives a two-page table on the transformation pressure of about 50 materials known up to 1994.

PIA types

- **True PIA**
  - a crystalline material that transforms (upon change of the external pressure) to a completely amorphous structure when a well defined transition pressure is reached.
- **Weak PIA**
  - A single-crystal sample transform to an X-ray amorphous state, e.g. a polycrystal with a sufficiently small crystal size. PRB 71, 224119 (2005)

Mechanism of PIA

- **Mechanical instability**: Most support it, e.g.
  - *elastic modulus* $= 0$: HDA ice Nature 384, 546–549 (1996); Nature 400, 647649 (1999); α quartz PRL 70, 174 (1993); PRE 52, 6484 (1995)
  - *soft phonon mode on the boundary of Brillouin zone* PRB 54, 12036 (1996)
  - *low-frequency vibrational rigid unit mode (RUM)*: ZrW_2O_8 Science 280, 886 (1998) Simultaneous softening a phonon branch along a direction in the Brillouin zone
- **Kinetically frustrated phase transition to another crystalline state** PRL 68, 3311 (1992); PRB 51, 11262 (1995)
- **Forming new chemical bonds**
  - amorphization of cubic $\mathrm{Ge_2Sb_2Te_5}$ is caused by the large displacement of Te atoms to the nearby vacancy position results into very strong Te-Te covalent bonds and Ge/Sb homopolar bonds PRL 102, 205502 (2009); PNAS 108, 10410 (2011) (simulation)
- **Bending of chemical bonds**
  - depressurization amorphization of single-crystal boron carbide (B_4C) is caused by "pressure-induced irreversible bending of C-B-C atomic chains cross-linking 12 atom icosahedra at the rhombohedral vertices." PRL 102, 075505 (2009) (experiments and simulation)

Abrupt vs. progressive transformation

Most are Abrupt

- ice I_h Nature 310, 393 (1984)

progressive

- ZrW_2O_8 Science 280, 8869 (1998) start at 1.5 GPa and complete at 3 GPa
- $Ge_2Sb_2Te_5$ PNAS 108, 10410 (2011) start at 18 GPa and complete at 22 GPa

Reversibility

Reversible: memory effect

- α-berlinite $AlPO_4$ Science 255, 1559 (1992)
- clathrate hydrate of tetrahydrofuran (THF) and sulphur hexafluoride, and THF zeolite JCP 94, 623 (1991); Nature 369, 724 (1994)
- ZrW_2O_8 annealed at 923K Science 280, 8869 (1998)
- $Ge_2Sb_2Te_5$ can recover at 145°C PNAS 108, 10410 (2011)
- $Co(OH)_2$ PRL 78, 1936 (1997) (only O-H bond is disordered)

Irreversible: can be stable when de-pressurized

- ice
- α quartz PRL 70, 174 (1993)
- ZrW_2O_8 at 300K Science 280, 8869 (1998)
- GeO_2 PRL 93, 115502 (2004)
- $Ge_2Sb_2Te_5$ can recover at 25°C PNAS 108, 10410 (2011)

The rigid unit (e.g. WO_4 and PO_4) is the key for reversibility

Is the structure the same as liquid?

Yes

- ice $\mathrm{I_h}$ Nature 310, 393 (1984)

Note: based on $g(r)$

No

- LDA and HDA ice Nature 400, 647 (1999)
  differ in local structure
- SiO_2 PRL 70, 174 (1993)
  "no structual relationships between pressure-amorphized quartz and silica glass"
- X-ray amorphous core-soften system PRB 71, 224119 (2005)

Is PIA low-temperature melting?

Yes

- ice $\mathrm{I_h}$ Nature 384, 546–549 (1996)
  crossover at 140-165 K: equilibrium melting $\rightarrow$ sluggish amorphization
- α-quartz and coesite Nature 334, 52 (1988)

No

- LDA and HDA ice Nature 400, 647 (1999)
  differ from liquid, indicating not melting
- α quartz PRL 70, 174 (1993)
  Anisotropy in PIA

Is PIA less studied now?

- **Yes, PIA is only a small subset of pressure-induced phase transformation.**
  - Hydrogen-riched high-pressure high-Tc superconductivity PRL 98, 117004 (2007); PRL 100, 045504 (2008); Nature 525, 73 (2015)
    SH_3: $T_c = 203$K at 90 GPa; AlH_3, SiH_4, SnH_4
    theory prediction: atomic phase metallic hydrogen $T_c =$ 300-350K at 500 GPa Rev. Mod. Phys. 84, 1607 (2012)
  - high pressure solid-solid transition: e.g., related to deep earthquakes PNAS 104, 9133 (2007), elements Phase Transformations of Elements Under High Pressure (2005)
- **No, PIA has many practical applications**
  - Boron carbide B_4C for armor
  - PIA-based phase-change random access memory $Ge_2Sb_2Te_5$ for fast reading/writing PRL 102, 205502 (2009); PNAS 108, 10410 (2011)
  - nanocrystalline alloys produced by crystallization of amorphous alloys Current Topics in Amorphous Materials: Physics & Technology (2013)

Periodic table

Period \ Group	1 Alkali metals	2 Alkaline earth metals	3		4	5	6	7	8	9	10	11	12	13	14	15 Pnictogens	16 Chalcogens	17 Halogens	18 Noble gases
1	Hydrogen 1 **H** 1.008																		Helium 2 **He** 4.0026
2	Lithium 3 **Li** 6.94	Beryllium 4 **Be** 9.0122												Boron 5 **B** 10.81	Carbon 6 **C** 12.011	Nitrogen 7 **N** 14.007	Oxygen 8 **O** 15.999	Fluorine 9 **F** 18.998	Neon 10 **Ne** 20.180
3	Sodium 11 **Na** 22.990	Magnesium 12 **Mg** 24.305												Aluminium 13 **Al** 26.982	Silicon 14 **Si** 28.085	Phosphorus 15 **P** 30.974	Sulfur 16 **S** 32.06	Chlorine 17 **Cl** 35.45	Argon 18 **Ar** 39.948
4	Potassium 19 **K** 39.098	Calcium 20 **Ca** 40.078	Scandium 21 **Sc** 44.956		Titanium 22 **Ti** 47.867	Vanadium 23 **V** 50.942	Chromium 24 **Cr** 51.996	Manganese 25 **Mn** 54.938	Iron 26 **Fe** 55.845	Cobalt 27 **Co** 58.933	Nickel 28 **Ni** 58.693	Copper 29 **Cu** 63.546	Zinc 30 **Zn** 65.38	Gallium 31 **Ga** 69.723	Germanium 32 **Ge** 72.630	Arsenic 33 **As** 74.922	Selenium 34 **Se** 78.971	Bromine 35 **Br** 79.904	Krypton 36 **Kr** 83.798
5	Rubidium 37 **Rb** 85.468	Strontium 38 **Sr** 87.62	Yttrium 39 **Y** 88.906		Zirconium 40 **Zr** 91.224	Niobium 41 **Nb** 92.906	Molybdenum 42 **Mo** 95.95	Technetium 43 **Tc** [98]	Ruthenium 44 **Ru** 101.07	Rhodium 45 **Rh** 102.91	Palladium 46 **Pd** 106.42	Silver 47 **Ag** 107.87	Cadmium 48 **Cd** 112.41	Indium 49 **In** 114.82	Tin 50 **Sn** 118.71	Antimony 51 **Sb** 121.76	Tellurium 52 **Te** 127.60	Iodine 53 **I** 126.90	Xenon 54 **Xe** 131.29
6	Caesium 55 **Cs** 132.91	Barium 56 **Ba** 137.33	Lanthanum 57 **La** 138.91	*	Hafnium 72 **Hf** 178.49	Tantalum 73 **Ta** 180.95	Tungsten 74 **W** 183.84	Rhenium 75 **Re** 186.21	Osmium 76 **Os** 190.23	Iridium 77 **Ir** 192.22	Platinum 78 **Pt** 195.08	Gold 79 **Au** 196.97	Mercury 80 **Hg** 200.59	Thallium 81 **Tl** 204.38	Lead 82 **Pb** 207.2	Bismuth 83 **Bi** 208.98	Polonium 84 **Po** [209]	Astatine 85 **At** [210]	Radon 86 **Rn** [222]
7	Francium 87 **Fr** [223]	Radium 88 **Ra** [226]	Actinium 89 **Ac** [227]	**	Ruther-fordium 104 **Rf** [267]	Dubnium 105 **Db** [268]	Seaborgium 106 **Sg** [269]	Bohrium 107 **Bh** [270]	Hassium 108 **Hs** [270]	Meitnerium 109 **Mt** [278]	Darm-stadtium 110 **Ds** [281]	Roentgenium 111 **Rg** [282]	Copernicium 112 **Cn** [285]	Nihonium 113 **Nh** [286]	Flerovium 114 **Fl** [289]	Moscovium 115 **Mc** [290]	Livermorium 116 **Lv** [293]	Tennessine 117 **Ts** [294]	Oganesson 118 **Og** [294]
				*	Cerium 58 **Ce** 140.12	Praseo-dymium 59 **Pr** 140.91	Neodymium 60 **Nd** 144.24	Promethium 61 **Pm** [145]	Samarium 62 **Sm** 150.36	Europium 63 **Eu** 151.96	Gadolinium 64 **Gd** 157.25	Terbium 65 **Tb** 158.93	Dysprosium 66 **Dy** 162.50	Holmium 67 **Ho** 164.93	Erbium 68 **Er** 167.26	Thulium 69 **Tm** 168.93	Ytterbium 70 **Yb** 173.05	Lutetium 71 **Lu** 174.97	
				**	Thorium 90 **Th** 232.04	Protactinium 91 **Pa** 231.04	Uranium 92 **U** 238.03	Neptunium 93 **Np** [237]	Plutonium 94 **Pu** [244]	Americium 95 **Am** [243]	Curium 96 **Cm** [247]	Berkelium 97 **Bk** [247]	Californium 98 **Cf** [251]	Einsteinium 99 **Es** [252]	Fermium 100 **Fm** [257]	Mendelevium 101 **Md** [258]	Nobelium 102 **No** [259]	Lawrencium 103 **Lr** [266]	

1 (red)=Gas 3 (black)=Solid 80 (green)=Liquid 109 (gray)=Unknown Color of the atomic number shows state of matter (at 0 °C and 1 atm)